

Rational Krylov Sequence Methods for Eigenvalue Computation

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ABSTRACT

Algorithms to solve large sparse eigenvalue problems are considered. A new class of algorithms which is based on rational functions of the matrix is described. The Lanczos method, the Arnoldi method, the spectral transformation Lanczos method, and Rayleigh quotient iteration all are special cases, but there are also new algorithms which correspond to rational functions with several poles. In the simplest case a basis of a rational Krylov subspace is found in which the matrix eigenvalue problem is formulated as a linear matrix pencil with a pair of Hessenberg matrices.

1. INTRODUCTION AND SUMMARY

The currently most successful iterative eigenvalue algorithms are built up around a Krylov subspace of vectors,

$$K^j(A, x_1) = \{x_1, Ax_1, \dots, A^{j-1}x_1\}. \quad (1.1)$$

The Lanczos [7] and Arnoldi [1] methods find an orthogonal basis of K^j . The subspace K^j is the space of polynomials of the matrix acting at the starting vector, and the theory of approximating polynomials is used to explain the behavior of algorithms based on the Krylov subspaces [4, 5, 11, 12, 15].

In practical applications inverse iterations are often of advantage, since by choosing appropriate shift points, they can be made to converge in very few iterations. Especially when the Lanczos method is used in the iteration, a very effective scheme can be developed [3]. Shifting and inverting corresponds to making a spectral transformation, using a rational function with pole at the shift point.

We now study methods which use arbitrary rational functions, with poles placed in an appropriate way. The work has just started, and we have no numerical results available. Several theoretical questions are also left open.

We continue in Section 2 with reviewing the theory of methods based on the Krylov subspaces, and in Section 3 we show how the theory of approximating polynomials is relevant for the study of the convergence of these methods. In Section 4 we describe how an iteration based on rational functions is carried out and which quantities are important when studying such an iteration. We conclude by reviewing possible applications in Section 5 and open questions in Section 6.

2. THE KRYLOV METHOD

Now let us recall the method of Krylov [6], and some of its modifications that are more appropriate from a numerical point of view.

Starting with an arbitrary vector x_1 , we compute a sequence of vectors,

$$x_{j+1} = Ax_j, \quad j = 1, 2, \dots \quad (2.1)$$

Denote by X_j the matrix formed by these vectors,

$$X_j = [x_1, x_2, \dots, x_j]. \quad (2.2)$$

The Krylov method relies on the fact that the vectors of the sequence (2.1) sooner or later become linearly dependent. Let us say that this happens at step p ($p \leq n$), i.e.

$$x_{p+1} = Ax_p = x_1 c_1 + \dots + x_p c_p = X_p c. \quad (2.3)$$

We see that

$$\begin{aligned} AX_p &= [Ax_1, \dots, Ax_p] \\ &= [x_2, \dots, X_p c] \\ &= X_p F_{pp}, \end{aligned} \quad (2.4)$$

where

$$F_{pp} = \begin{bmatrix} 0 & 0 & \cdots & c_1 \\ 1 & 0 & \cdots & c_2 \\ 0 & 1 & \cdots & c_3 \\ 0 & 0 & \cdots & c_p \end{bmatrix}$$

is a Frobenius (or companion) matrix of order $p \times p$.

The eigenvalues of F are a subset of the eigenvalues of A , and F has the characteristic polynomial

$$\chi_{F_{pp}}(\lambda) \equiv \lambda^p - c_p \lambda^{p-1} - c_{p-1} \lambda^{p-2} - \cdots - c_1.$$

In a numerical application, it is not possible to determine p in a precise fashion, but linear dependence occurs gradually. Instead of the equality (2.3), we get a residual

$$r_{p+1} = Ax_p - X_p c, \quad (2.5)$$

and also (2.4) will be replaced by a difference,

$$AX_p - X_p F_{pp} = r_{p+1} e_p^T, \quad (2.6)$$

and we note that the difference has only its last column filled with elements:

$$r_{p+1} e_p^T = \begin{bmatrix} 0 & 0 & \cdots & \rho_1 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & \rho_n \end{bmatrix}.$$

The eigenvalues of F_{pp} are now approximations to the eigenvalues of A . Let μ, s be an eigenpair of F :

$$Fs = s\mu.$$

Then μ is an approximate eigenvalue, and

$$y = X_p s,$$

will be an approximate eigenvector to A . The residual will be

$$\begin{aligned} Ay - y\mu &= AX_p s - X_p F s \\ &= (AX_p - X_p F) s \\ &= r_{p+1} e_p^T s = r_{p+1} s(p), \end{aligned} \quad (2.7)$$

the product of the residual vector and the last component of the eigenvector s of F .

We have not yet determined the linear combination c , which partly determines r_{p+1} . One natural choice is the one that gives the residual r_{p+1} in (2.5), (2.6), (2.7) a minimal norm. Then we get c from (2.5) as the solution to a linear least squares problem, with X_p as its matrix and Ax_p as right hand side, making

$$X_p^H r_{p+1} = 0.$$

We choose the last column c of F so that the residual r_{p+1} is orthogonal to the Krylov subspace spanned by X_p .

We note that the eigenvalue and eigenvector approximation is entirely determined by the subspace $\text{span}\{X_p\}$ and the direction of the residual r_{p+1} . It is therefore possible to choose another basis for the subspace, and a natural choice is to apply the orthogonalization process at every step $j = 1, 2, \dots, p$. We then get a Hessenberg matrix

$$H_{pp} = \begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1p} \\ h_{21} & h_{22} & \cdots & h_{2p} \\ 0 & h_{32} & \cdots & h_{3p} \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & h_{pp} \end{bmatrix}$$

instead of F_{pp} . This is the Arnoldi method [1]. It gives an orthogonal basis of the Krylov subspace. If furthermore A is symmetric, so is H_{pp} , since by (2.6) (X_p is orthogonal now)

$$\begin{aligned} H_{pp} &= X_p^H A X_p, \\ H_{pp}^H &= X_p^H A^H X_p = H_{pp}, \end{aligned}$$

and we get the Lanczos algorithm [7].

We note that the expression for the residual, in terms of last elements of eigenvectors, is entirely parallel to that for the Lanczos method (see e.g. [12]). The importance of the last column of the matrix for the direction of the residual was noted by Saad [16].

The linear dependence of the Krylov sequence has been used numerically by Manteuffel [8] and Saylor [17]. They use the case $p = 2$ to determine a complex leading eigenvalue of a slowly convergent sequence of vectors.

3. POLYNOMIALS OF A

We will now describe how the theory of the Krylov sequence can be given in terms of polynomials of the matrix, and how the theory of approximation by polynomials can be used to explain the convergence of methods based on the Krylov sequence.

Every vector in the Krylov subspace,

$$y \in K^j(A, x_1) \equiv \{x_1, \dots, x_j\}, \quad (3.1)$$

can be written as a polynomial

$$y = X_j c = \eta(A) x_1$$

with the polynomial

$$\eta(\lambda) = c_j \lambda^{j-1} + c_{j-1} \lambda^{j-2} + \dots + c_1$$

of degree $j - 1$. Recall from the last section that the approximate eigenvector $y \in K^p(A, x_1)$ satisfies (2.7):

$$Ay - y\mu = s(p)r_{p+1} \perp K^p(A, x_1). \quad (3.2)$$

By (2.3) we see that

$$r_{p+1} = \chi_p(A)x_1.$$

Denote

$$y = \eta(A)x_1, \quad (3.3)$$

and let

$$z = \zeta(A)x_1$$

be an arbitrary vector in $K^p(A, x_1)$. Then by (3.2)

$$(\zeta(A)x_1)^H \chi_p(A)x_1 = 0.$$

In the symmetric case this means that

$$x_1^H \zeta(A) \chi_p(A)x_1 = 0.$$

The successive characteristic polynomials χ_p are orthogonal polynomials with respect to the scalar product

$$\langle \xi, \eta \rangle \equiv \int \xi(\lambda) \eta(\lambda) d\alpha(\lambda), \quad (3.4)$$

with the integrator $d\alpha$ having weights α_i^2 at the eigenvalues λ_i ; the α_i are the expansion coefficients of the starting vector in terms of the eigenvectors of A :

$$\begin{aligned} x_1 &= u_1 \alpha_1 + \cdots + u_n \alpha_n, \\ u_1, \dots, u_n &\text{ eigenvectors of } A. \end{aligned}$$

Moreover the eigenvector approximation (3.3) is given by the quotient

$$\eta(\lambda) = \frac{\chi_p(\lambda)}{\lambda - \mu}.$$

The relation between the Krylov sequence and the integrator (3.4) was expounded in Hestenes and Stiefel [4], and has been used to give *a priori* results on the convergence of the Lanczos method by Kaniel [5], Paige [11], and Saad [15].

4. RATIONAL FUNCTIONS OF A

The Krylov subspace

$$K^j(A, x_1) = \{x_1, Ax_1, \dots, A^{j-1}x_1\} \quad (4.1)$$

was spanned by the powers of A , and every vector in it could be expressed as a polynomial. Let us now see what happens when we take an arbitrary set of basis functions, and then investigate easily computable sets of rational functions.

Let $\varphi_1, \varphi_2, \dots, \varphi_j$ be any sequence of functions, and consider the sequence of vectors

$$F_j(A, x_1) = \{ \varphi_1(A)x_1, \varphi_2(A)x_1, \dots, \varphi_j(A)x_1 \}. \quad (4.2)$$

If we increase j , we will also now sooner or later get a linear dependence among these vectors, let us say

$$\varphi_1(A)x_1c_1 + \dots + \varphi_p(A)x_1c_p = 0. \quad (4.3)$$

In order to see how (4.3) can be used to compute eigenvalues of A , we expand the starting vector x_1 in terms of the eigenvectors u_i of A (disregard the defective case for the moment),

$$x_1 = Ua = u_1\alpha_1 + \dots + u_n\alpha_n. \quad (4.4)$$

We see that

$$\begin{aligned} \varphi_j(A)x_1 &= u_1\varphi_j(\lambda_1)\alpha_1 + \dots + u_n\varphi_j(\lambda_n)\alpha_n \\ &= U \operatorname{diag}(\varphi_j(\lambda_i)) a. \end{aligned} \quad (4.5)$$

Use (4.5) to expand the linear dependence (4.3) in terms of eigenvectors, and get

$$\begin{aligned} 0 &= U \operatorname{diag}(\varphi_1(\lambda_i)) ac_1 + \dots + U \operatorname{diag}(\varphi_p(\lambda_i)) ac_p \\ &= U \{ \operatorname{diag}(\varphi_1(\lambda_i)) c_1 + \dots + \operatorname{diag}(\varphi_p(\lambda_i)) c_p \} a \\ &= U \operatorname{diag}(\phi(\lambda_i)) a. \end{aligned} \quad (4.6)$$

The linear combination

$$\phi(\lambda) = c_1\varphi_1(\lambda) + \cdots + c_p\varphi_p(\lambda),$$

will thus have zeros at those eigenvalues that are represented in the starting vector.

In a numerical case we do not get exactly zero in (4.3). We can seek an approximate linear dependence using the singular value decomposition,

$$X_p = U_p \Sigma_p V_p^H$$

and see that for $c = v_p$, the right singular vector corresponding to the smallest singular value, we have

$$X_p c = \sigma_p u_p$$

giving the (normalized) linear combination with the smallest residual. With this c we have

$$\begin{aligned} \phi(A)x_1 &= r_p, \\ r_p &= \sigma_p u_p. \end{aligned} \tag{4.7}$$

If μ_i is a zero of $\phi(\lambda)$, we can write

$$\phi(\lambda) = (\lambda - \mu_i)\Psi(\lambda), \tag{4.8}$$

and take

$$y = \frac{\Psi(A)x_1}{\|\Psi(A)x_1\|}, \tag{4.9}$$

as an approximate eigenvector. Its residual is given by

$$\begin{aligned} Ay - y\mu_i &= \frac{(A - \mu_i I)\Psi(A)x_1}{\|\Psi(A)x_1\|} \\ &= \frac{\phi(A)x_1}{\|\Psi(A)x_1\|} \\ &= \frac{\sigma_p u_p}{\|\Psi(A)x_1\|}, \end{aligned} \tag{4.10}$$

and we see that we get a small residual when σ_p is small (the sequence is close to linear dependence) or $\|\Psi(A)x_1\|$ is large ($\phi(\lambda)$ has a steep slope at the zero). Note that (4.10) is independent of a multiplication of the c_i in (4.3) by a constant. We should therefore aim at finding a sequence φ_j such that a linear combination is likely to have steep slopes at its zeros.

Let us now turn to the basis functions $\varphi_1, \dots, \varphi_p, \dots$. Besides polynomials, which we have already treated, the only feasible choice computationally is rational functions. The algorithm has to choose where the poles are situated in the complex plane, while the zeros will yield eigenvalue approximations. The closer the poles are to the zeros, the steeper will the slopes be and the better the approximations. We choose to represent the rational functions as cumulative partial fractions

$$r_p(\lambda) = \frac{p_p(\lambda)}{q_p(\lambda)} = c_1 + \frac{c_2}{(\lambda - \mu_1)} + \dots + \frac{c_{p+1}}{(\lambda - \mu_1) \cdots (\lambda - \mu_p)}. \quad (4.11)$$

It is well known that any rational function with equal degree in numerator and denominator and poles in μ_1, \dots, μ_p can be written in this way. Repeated poles cause no problem. We see that the representation (4.11) corresponds to the choice of basis functions,

$$\begin{aligned} \varphi_1 &= 1, \\ \varphi_{k+1} &= \frac{\varphi_k}{\lambda - \mu_k}, \quad k = 1, \dots, p, \end{aligned} \quad (4.12)$$

and that the basis vectors x_1, \dots, x_{p+1} are computed as

$$\begin{aligned} x_1 &= \text{starting vector}, \\ x_{k+1} &= (A - \mu_k I)^{-1} x_k, \end{aligned} \quad (4.13)$$

i.e. as an inverse iteration with possibly varying shifts.

In order to find eigenvalue approximations we need a convenient way of determining the zeros of a function represented as (4.11). We see that $r_p(\lambda)$

can be computed by the recursion

$$r_{p+1} = c_{p+1},$$

$$r_k = \frac{r_{k+1}}{\lambda - \mu_k} + c_k, \quad k = p, \dots, 1;$$

$$r_1 = r_p(\lambda),$$

which is an expansion of the determinant

$$r_p(\lambda) = \det \begin{bmatrix} \frac{1}{\lambda - \mu_1} & 0 & \cdots & 0 & c_1 \\ -1 & \frac{1}{\lambda - \mu_2} & \cdots & 0 & c_2 \\ 0 & -1 & \cdots & 0 & c_3 \\ 0 & 0 & \cdots & \frac{1}{\lambda - \mu_p} & c_p \\ 0 & 0 & \cdots & -1 & c_{p+1} \end{bmatrix}. \quad (4.14)$$

Each column describes how we find the next vector in the sequence (4.13), and the last one is the linear combination.

The linear combination is determined up to a constant factor; let us assume that $c_{p+1} = 1$. Then (4.14) can be replaced by a $p \times p$ determinant

$$r_p(\lambda) = \det \begin{bmatrix} \frac{1}{\lambda - \mu_1} & 0 & \cdots & c_1 \\ -1 & \frac{1}{\lambda - \mu_2} & \cdots & c_2 \\ 0 & -1 & \cdots & c_3 \\ 0 & 0 & \cdots & \frac{1}{\lambda - \mu_p} + c_p \end{bmatrix},$$

which is the rational analogue of the Frobenius matrix.

As in the case of the Krylov method, it is natural to consider successive orthogonalization and replace (4.13) by the rule

$$\begin{aligned} x_1 &= \text{starting vector}, \quad \|x_1\| = 1, \\ h_{k+1k}x_{k+1} &= (A - \mu_k I)^{-1}x_k - h_{1k}x_1 - \cdots - h_{kk}x_k, \end{aligned} \quad (4.15)$$

yielding a rational Hessenberg matrix

$$\begin{bmatrix} \frac{1}{\lambda - \mu_1} - h_{11} & -h_{12} & \cdots & -h_{1p} \\ -h_{21} & \frac{1}{\lambda - \mu_2} - h_{22} & \cdots & -h_{2p} \\ 0 & & \ddots & \vdots \\ \vdots & & & \frac{1}{\lambda - \mu_p} - h_{pp} \\ 0 & \cdots & 0 & -h_{p+1p} \end{bmatrix}.$$

On convergence $h_{p+1p} = 0$, and we get a generalized eigenproblem, which can be treated by the QZ algorithm [9]. Multiply each column by $\lambda - \mu_k$ and get

$$r_p(\lambda) = \frac{1}{(\lambda - \mu_1) \cdots (\lambda - \mu_p)} \det(K - \mu L), \quad (4.16)$$

where

$$\begin{aligned} K &= I + HM, \\ L &= H \end{aligned}$$

with

$$H = \begin{bmatrix} h_{11} & \cdots & h_{1p} \\ h_{21} & \cdots & h_{2p} \\ 0 & \cdots & h_{pp} \end{bmatrix},$$

$$M = \text{diag}(\mu_k).$$

Note that H , as well as K and L , is built up one column at a time, so that we

can proceed step by step, until we get sufficiently good eigenvalue approximations, precisely as in the case of the Lanczos or the Arnoldi algorithm.

In the real nonsymmetric case, rational functions with denominators of second degree are interesting, since they give a possibility of using complex shifts in real arithmetic. That case can also be reduced to a linear problem (4.16), but now with block Hessenberg matrices K and L , with 2×2 blocks whenever a second degree factor is used. We do not give the details of that procedure here.

5. APPLICATIONS

We have as of now no practical experience of algorithms based on the rational Krylov concept, but there are some obvious cases where we believe they will be of advantage.

Consider first large symmetric problems typically arising from finite element computations. The currently best algorithms for those problems [3, 10, 18] make a sequence of spectral transformations with shifts μ_1, μ_2, \dots . For each μ a shifted and inverted matrix

$$(A - \mu I)^{-1} \quad (5.1)$$

is used in a Lanczos algorithm. When a new shift is used, the Lanczos method is restarted. In the strategy given in [3], each Lanczos run goes $p = 20$ –40 steps. Usually no eigenvalues converge for the first 10 steps, but then they fall in at the rate of about two every five steps. The dominating cost of the algorithm is the matrix-vector multiplication using a factorized version of (5.1).

With the rational recursion (4.13), we can now change shifts during one run. This will save us iterations, at the cost of having a Hessenberg problem (4.16), instead of the tridiagonal matrix from Lanczos, to analyze at each step. Changing shifts more often should be most advantageous for problems where the cost of factorization is modest compared to the cost of 10 solution steps, i.e. for very sparse problems, where a fast Poisson solver or a multigrid algorithm is used for the solution. See [2] for a review of special methods for sparse linear systems.

The second application that comes to mind is Rayleigh quotient iteration (see [12]). Here we iterate

$$x_{s+1} = (A - \mu_s I)^{-1} x_s,$$

and we see that it corresponds to (4.13)

The sequence μ_s converges very fast towards one eigenvalue, so it is not likely that we will get a faster convergence by studying linear combinations, but we can use the vectors computed to get an approximation to another eigenvalue. This will start a new sequence of μ_s converging to that second eigenvalue, and so on.

The third application is for nonsymmetric problems. Those are likely to be more difficult to treat, since we have no simple criterion like the inertia count available, to determine whether all sought-after eigenvalues have been found. We can then place shifts in interesting parts of the complex plane, and get accurate determinations of eigenvalues close to those shifts. If we have an indication of an eigenvalue at a certain position, we can shift there and determine it accurately. In typical cases, the region around the imaginary axis is of special interest when determining the stability of a dynamical system. Note that in the nonsymmetric case an algorithm based on a single spectral transformation like Arnoldi's [14] takes about the same computational effort, since then also a Hessenberg matrix is generated.

6. FUTURE WORK

As stated in the introduction, the work of developing algorithms based on the rational Krylov method has just started. There are several subproblems that need to be studied.

One of them is to develop a minimality theory for rational functions, usable in the same way as the minimality of Chebyshev polynomials is used, for methods based on the Krylov sequence. The rational functions we deal with are special in that the denominators have to be determined during the computation, while the numerators are free. To get an *a priori* bound, usable in conjunction with (4.10), we seek solutions to the minimax problem (\mathbb{P}^n is the set of polynomials of degree n)

$$\min_{\substack{p \in \mathbb{P}^j \text{ monic} \\ q \in \mathbb{P}^k \text{ given}}} \max_{\lambda \in \{\lambda_1, \dots, \lambda_n\}} \left| \frac{p(\lambda)}{q(\lambda)} \right|. \quad (6.1)$$

We see that it is more complicated than in the polynomial case, since we cannot replace the discrete set $\lambda_1, \dots, \lambda_n$ by an interval. It is likely that $q(\lambda)$ has zeros interlacing the λ_i 's, giving $r(\lambda) = p(\lambda)/q(\lambda)$ poles there. The denominator of (4.10) is essentially the derivative of $r(\lambda)$, i.e., we seek an $r(\lambda)$ with steep slopes at the zeros.

Another open question is how symmetry will show up during the computation. Evidently (4.16) will not in general be symmetric. If the shift μ_k is kept constant for several steps, the corresponding subblock of K and L will form a symmetric problem; e.g., when we run with two different shifts, we will get

$$H = \left[\begin{array}{c|c} T_j & H_{jp-j} \\ \hline h_{j+1j} & T_{p-j} \\ 0 & \end{array} \right],$$

with T_j and T_{p-j} tridiagonal, and K and L correspondingly so, yielding two coupled tridiagonal symmetric eigenproblems.

An interesting algorithmic detail is how to obtain solutions for successively expanding $K - \lambda L$ problems (4.16). There are methods for expanding tridiagonal matrices [13], but the Hessenberg case will be a little bit more complicated.

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